

# Sparse random matrix configurations for two or three interacting electrons in a random potential

*Shi-Jie Xiong<sup>1,2</sup> and S.N. Evangelou<sup>1,3</sup>*

<sup>1</sup>*Foundation for Research and Technology,*

*Institute for Electronic Structure and Lasers,*

*Heraklion, P.O. Box 1527, 71110 Heraklion, Crete, Greece*

<sup>2</sup>*Department of Physics, Nanjing University,*

*Nanjing 210008, China*

<sup>3</sup>*Department of Physics, University of Ioannina,*

*Ioannina 451 10, Greece*

## **Abstract**

We investigate the random matrix configurations for two or three interacting electrons in one-dimensional disordered systems. In a suitable non-interacting localized electron basis we obtain a sparse random matrix with very long tails which is different from a superimposed random band matrix usually thought to be valid. The number of non-zero off-diagonal matrix elements is shown to decay very weakly from the matrix diagonal and the non-zero matrix elements are distributed according to a Lorentzian around zero with also very weakly decaying parameters. The corresponding random matrix for three interacting electrons is similar but even more sparse.

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There is a great current interest in the localization weakening effect due to the interaction of two electrons in one-dimensional (1D) disordered systems [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]. Shepelyansky [1] mapped this problem onto a class of random banded matrices with strongly fluctuating diagonal elements, being the eigenenergies of the non-interacting problem, and independent Gaussian random off-diagonal matrix elements of zero average and typical strength  $\frac{U}{\xi_1^{3/2}}$ , lying in a band of width the one particle localization length  $\xi_1$  with  $U$  the strength of the interaction. Moreover, by the mapping to a superimposed banded random matrix ensemble (*SBRM*) a fraction of  $\frac{\xi_1}{2L}$  states with a considerable enhancement  $\xi \sim U^2 \xi_1^2$  of the localization length along the center of mass coordinate is predicted due to coherent propagation of the electronic pair. It was also shown that the interaction has no effect for the majority of other states with the two particles localized in isolated spatial positions which do not allow overlapping. This conclusion was confirmed and extended to higher dimensions via Thouless block scaling picture by Imry [2]. The subsequent numerical studies [3, 4, 5, 6, 7, 8, 9, 10] verified the main qualitative results concerning the presence of Shepelyansky states, mostly by suppressing single particle transport via efficient Green function or bag model methods which examine pair propagation [8]. The deviations from the predicted behavior of the two-particle localization length  $\xi$  found were usually attributed to the oversimplified statistical assumptions concerning the band random matrix model of the original Shepelyansky construction.

However, there is an ongoing debate whether coherent pair propagation actually exists for two interacting electrons in infinite disordered systems [11, 12], which began by a recent transfer matrix study where no propagation enhancement is found at  $E = 0$  for an infinite chain [11]. Moreover, it was pointed out that the reduction to a *SBRM* relies on questionable assumptions regarding chaoticity of the non-interacting electron localized states within  $\xi_1$ , so that the relevant matrix model could be prob-

ably different [13, 14]. Although the reported absence of propagation enhancement [11] can be criticized, since the transfer matrix method may not measure the actual pair localization length, it is correct that the fraction of the Shepelyansky states will eventually shrink to zero when the system size increases, although not affecting their physical significance. A different localization length enhancement for these states, of the form  $\xi \sim U^2 \xi_1^{1+\gamma}$  with a  $U$ -dependent exponent  $\gamma < 1$ , was also proposed on the basis of numerical data by a reduction mechanism to another appropriate random matrix model [13]. It must be mentioned that the Shepelyansky states are expected to exist as long as the interaction is not too large, since it is firmly established [10, 13] that in the strong interaction limit  $U \rightarrow \infty$  no coherent propagation enhancement is possible with these states decoupled from the main band with  $\xi \approx \xi_1$ .

It is worthwhile to check the validity of the mapping to a *SBRM* which allowed most of the previous results concerning the Shepelyansky states to be derived. The fact that a mapping to *SBRM* neglects phase correlations of the one particle localized states was also emphasised for a few known examples in another recent study [14], where it led to a non-justified propagation enhancement. In order to shed light on the appropriate random matrix description for the problem of two interacting electrons in a random potential we examine explicitly the structure of the two and three-electron Hamiltonian matrices by a direct numerical analysis. The corresponding Anderson-Hubbard Hamiltonian[15, 16] can be written as

$$\begin{aligned}
H = & \sum_{n=1}^N \sum_{\sigma} (c_{n+1,\sigma}^{\dagger} c_{n,\sigma} + \text{H.c.}) + \sum_{n=1}^N \sum_{\sigma} \epsilon_n c_{n,\sigma}^{\dagger} c_{n,\sigma} \\
& + \sum_{n=1}^N \sum_{\sigma \neq \sigma'} U c_{n,\sigma'}^{\dagger} c_{n,\sigma'} c_{n,\sigma}^{\dagger} c_{n,\sigma},
\end{aligned} \tag{1}$$

where  $c_{n,\sigma}^{\dagger}$  and  $c_{n,\sigma}$  are the creation and destruction operators for the electron at site  $n$  and with spin  $\sigma$ ,  $\epsilon_n$  is energy level at site  $n$  which is a random variable uniformly

distributed in the range  $[-W/2, W/2]$  as for the Anderson model and  $U$  is the strength of the interaction between the electrons.

A non-interacting disordered system of  $N$  atoms with  $U = 0$  in Eq. (1) has  $N$  linearly independent one-electron localized wave functions  $\psi_i$  with corresponding eigenvalues  $E_i$ ,  $i = 1, 2, 3, \dots, N$ . These exponentially localized wave functions are of the approximate form

$$\psi_i(n) \sim \frac{1}{\sqrt{\xi_1}} \exp \left[ -\frac{|n - n_i|}{\xi_1} + i\theta_i(n) \right], \quad (2)$$

where  $n_i$  is the localization center of  $\psi_i$  and  $\theta_i$  a corresponding phase factor. The corresponding perturbational localization length for small  $W$  is  $\xi_1 \approx \frac{96-24E^2}{W^2}$  where  $E$  is the single particle energy, although for some special  $E$  the prefactor is different. In order to examine the few-body problem in the presence of disorder we have obtained numerically all the localized states  $\psi_i$  and arranged them so that if  $i < j$  the coordinate  $n_i$  for the localization center of  $\psi_i$  is smaller than the corresponding center  $n_j$  of the wave function  $\psi_j$ . This is a natural kind of arrangement which guarantees the largest overlapping of the wave functions to occur when their indices have the smallest difference.

Firstly, we consider two electrons with opposite spins and use the  $N^2$  products of the two one-electron wave functions

$$\Psi_m^{(2)} = \psi_i \psi_j, \quad i, j = 1, 2, \dots, N, \quad (3)$$

as convenient basis states for the two interacting electrons. We do not consider the spin configuration of the two-electron wave function as suggested in Ref. [1]. The index  $m$  is also arranged in such a way so that states with the smallest difference of their indices have the strongest coupling. One can calculate the matrix elements of the  $U$ -dependent Hubbard interaction term of Eq. (1) in the obtained new basis set

via

$$H_{m,m'} = U \sum_n \psi_i(n) \psi_j(n) \psi_{i'}(n) \psi_{j'}(n). \quad (4)$$

In the original *SBRM* construction the matrix element  $H_{m,m'}$  was shown to vanish unless all four relevant wave functions were overlapping. Then each  $\psi_i(n)$  was assumed completely random within  $\xi_1$  by taking the approximate states of Eq. (2) with a random phase factor  $\theta_i(n)$ , so that one immediately obtains the estimate  $\frac{U}{\xi_1^{3/2}}$  for the typical magnitude of the off-diagonal matrix elements distributed within a band range. The *SBRM* construction ignores phase correlations which are known to give regular or fast oscillations within  $\xi_1$  for the single particle localized wave functions.

In Figs. 1 and 2 we show the obtained distribution of the diagonal and the off-diagonal matrix elements for two interacting electrons with disorder extent  $W$  and interaction strength  $U$ . The diagonal matrix elements are seen to obey a Gaussian distribution as expected. The off-diagonal matrix elements are found to be mostly zero but also very close to zero with a Lorentzian distribution having very long tails in the latter case. In order to fit the obtained distribution for the off-diagonal matrix elements  $h$  in the adopted basis we use the following function sum

$$f(h) = f_G(h) + f_L(h) = a_1 \exp\left(-\frac{1}{a_2} h^2\right) + \frac{a_3}{h^2 + a_4}, \quad (5)$$

where the Gaussian-like term  $f_G$  accounts for the distribution of the off-diagonal elements which are very close to zero and the Lorentzian-like term  $f_L$  for the long tails. The variations of the obtained four fitting parameters  $a_1$ ,  $a_2$ ,  $a_3$  and  $a_4$  as a function of the distance of the matrix element locations from the main matrix diagonal are shown to decay extremely weakly in Figs. 3 and 4. It can immediately be seen that  $a_1$  is much larger than  $a_3$  which implies a very large number of near-zero matrix elements. The obtained parameters  $a_2, a_4$  characterising the distribution are found very small.

We have also investigated the random matrix structure for the corresponding three electron problem. In order to simplify the calculations we have restricted our consideration to three electrons where two of them have spin up and one spin down. For a chain of  $N$ -sites in the adopted three-electron basis there are  $N^2(N - 1)/2$  linearly independent states whose wave functions can be written as

$$\Psi_m^{(3)} = \psi_{i,\uparrow}\psi_{j,\uparrow}\psi_{k,\downarrow}, \quad i \neq j. \quad (6)$$

We again sort these 3-particle states in such a way so that those with the smallest difference in their indices have the strongest possible coupling. In Fig. 5 we display the obtained distributions for the diagonal and the off-diagonal matrix elements. For the diagonal elements the distribution is more sharp when compared to the two-electron case, reflecting a smearing effect in the total energy fluctuations due to the increase in the number of particles. We find that the off-diagonal matrix elements obey the general principles of the two-electron problem but the matrix structure is comparatively even more sparse in this case.

In summary, we have studied the random matrix configurations for two or three interacting electrons in a disordered chain. We made a basis set arrangement which consists of non-interacting particle wave function products of orbitals so that the off-diagonal matrix elements due to the interaction occur successively only for states having closely spaced indices. Although this is the most favourable basis set for obtaining a *SBRM* a very sparse random matrix structure is shown to emerge from our data instead, having no well-defined band region with Gaussian matrix elements. We think finding another basis set consistent with a band random matrix structure is not easy and the few-body problem can be studied via extremely sparse random matrix configurations. It must be pointed out that the obtained sparse matrix is not incompatible with states having enhanced localization length along the center

of mass coordinate, since they can be shown by methods which do not rely on the specific matrix mapping [8, 17].

## **Acknowledgments**

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## Figure Captions

**Fig. 1.** The distribution of the matrix elements for the two-electron Hamiltonian with disorder  $W = 3$ , interaction strength  $U = 1$  and chain size  $N = 100$ . **(a)** The diagonal matrix elements. **(b)** The first off-diagonal matrix elements (continuous line) and the fitting curve from Eq. (5) (broken line).

**Fig. 2.** The same as Fig. 1 but for  $W = 6$  and interaction strength  $U = 4$ .

**Fig. 3.** The four fitting parameters  $a_1, a_2, a_3, a_4$  of Eq. (5) for the distribution of the off-diagonal matrix elements corresponding to Fig. 1 as a function of the distance from the main matrix diagonal, with chain size  $N = 100$ , disorder  $W = 3$  and interaction strength  $U = 1$ .

**Fig. 4.** The same as Fig. 3 but for  $W = 6$  and interaction strength  $U = 4$  corresponding to Fig. 2.

**Fig. 5.** The distribution of the matrix elements for the three-electron Hamiltonian with disorder  $W = 6$ , interaction strength  $U = 4$  and chain size  $N = 100$ . **(a)** The distribution of the diagonal matrix elements. **(b)** The distribution of the first off-diagonal matrix elements.

Fig. 1(a)

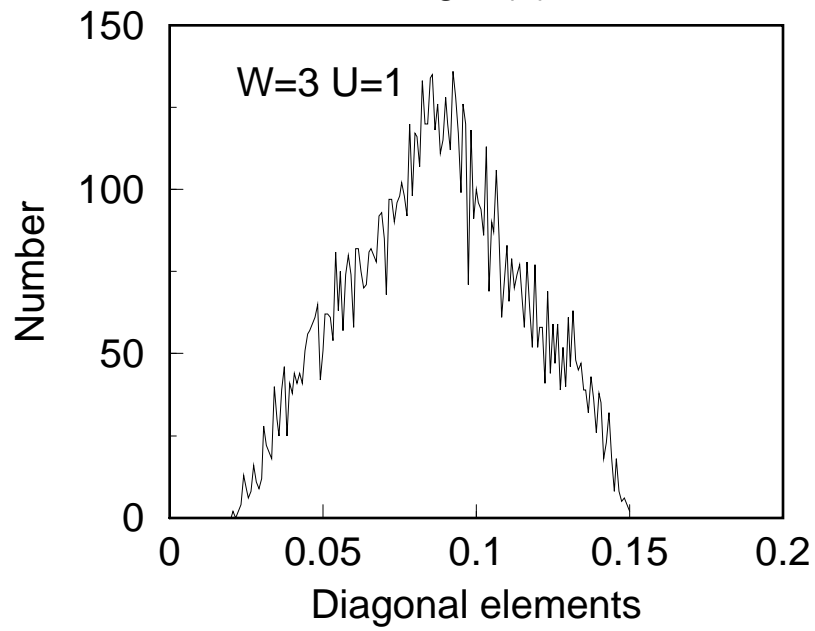


Fig. 1(b)

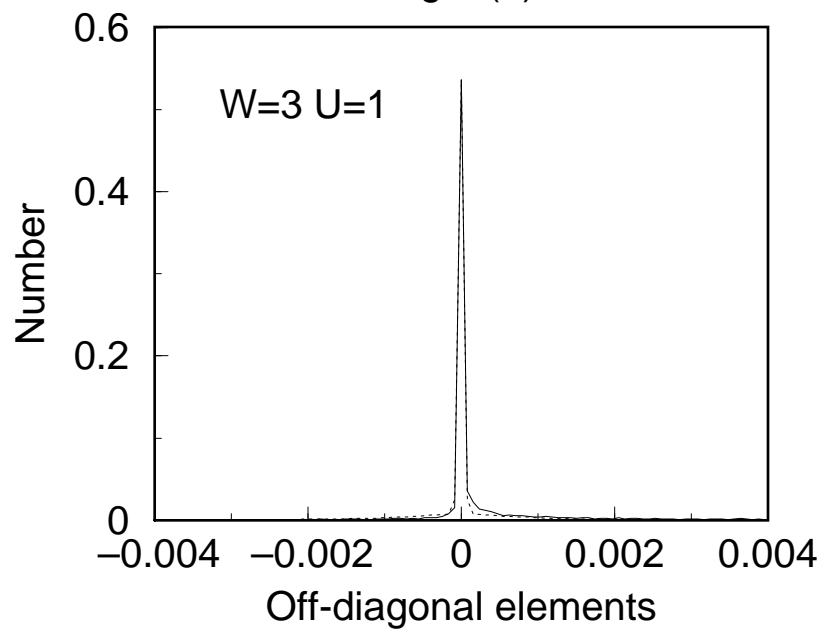


Fig. 2(a)

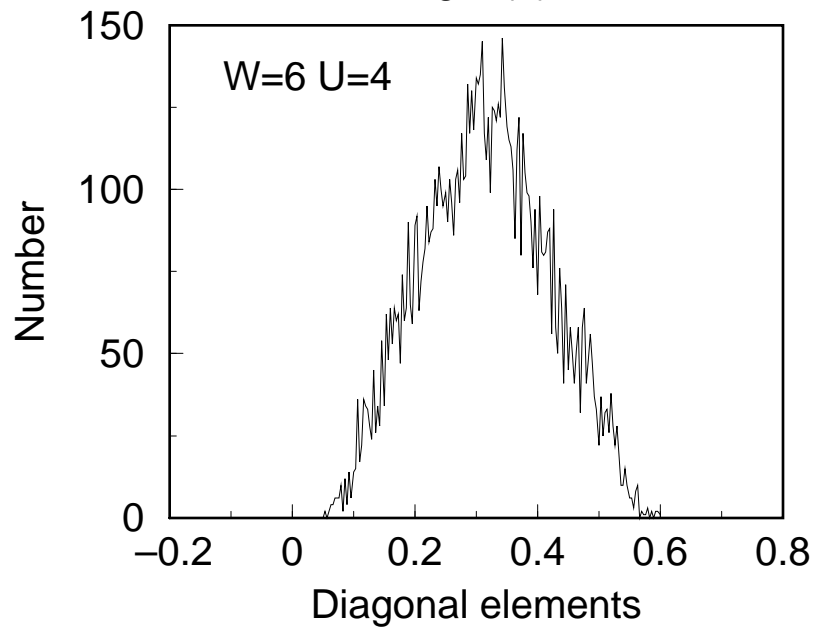


Fig. 2(b)

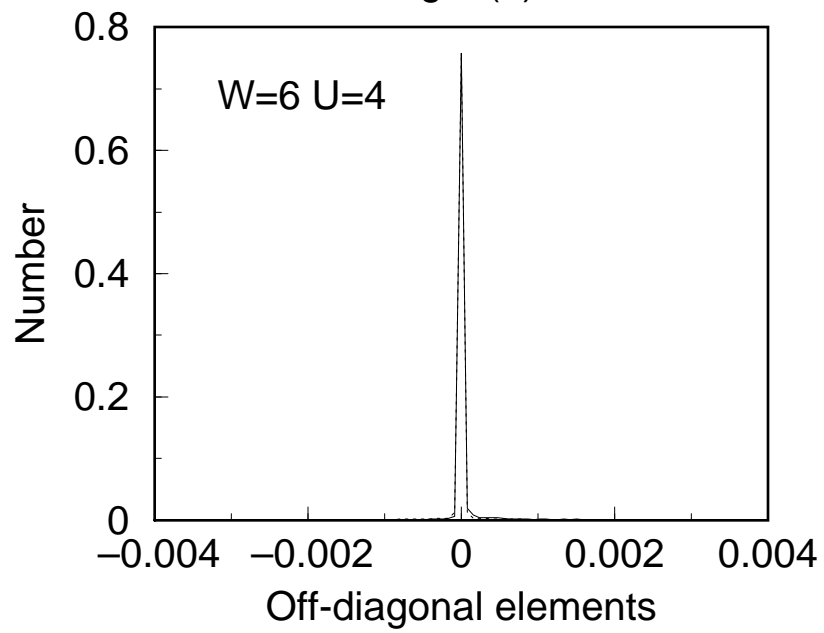


Fig. 3(a)

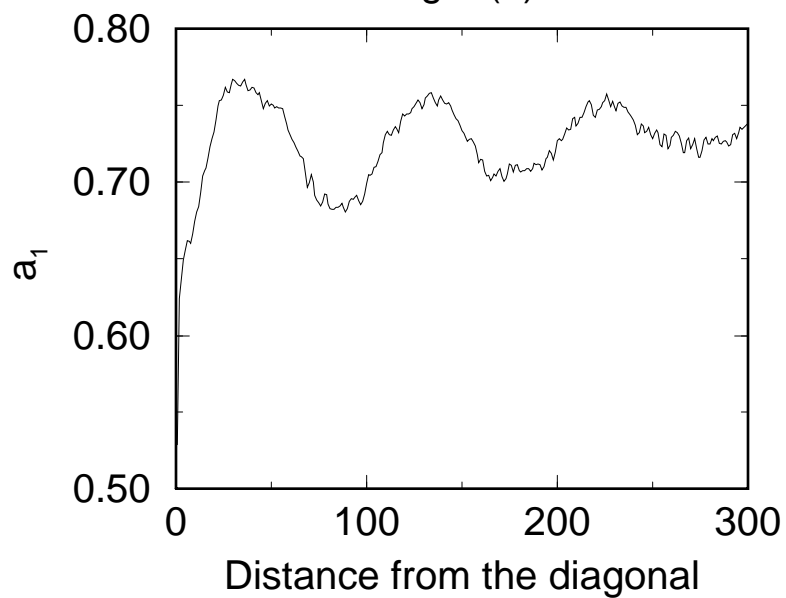


Fig. 3(b)

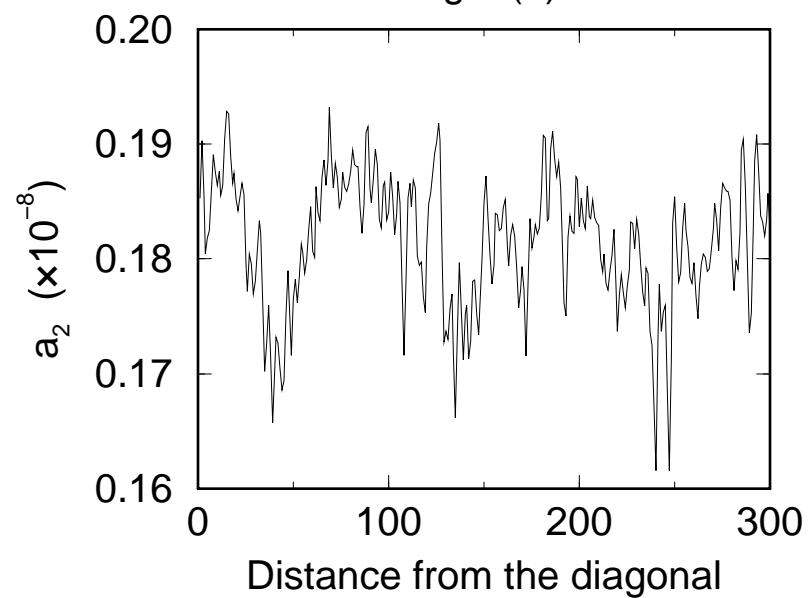


Fig. 3(c)

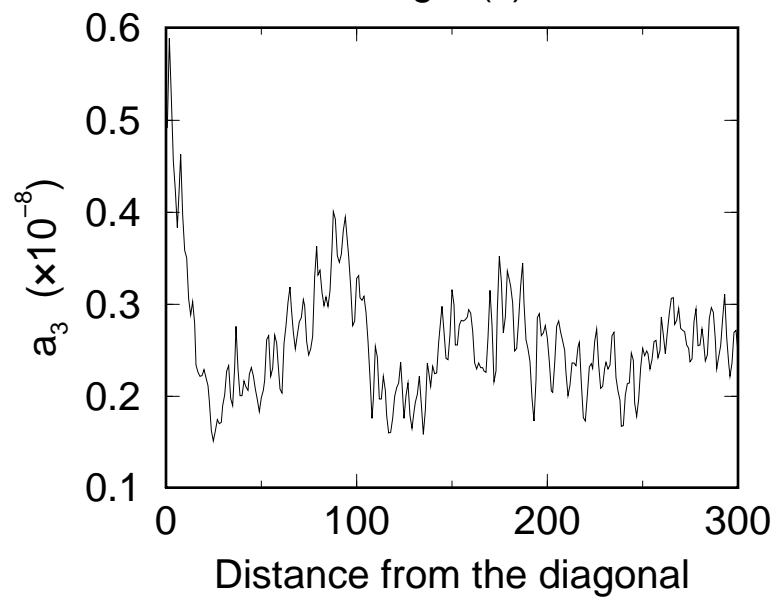


Fig. 3(d)

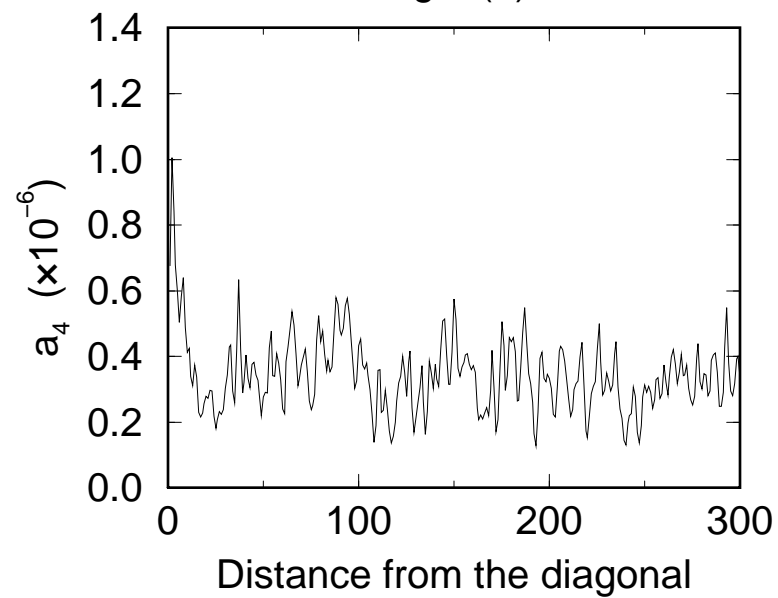


Fig. 4(a)

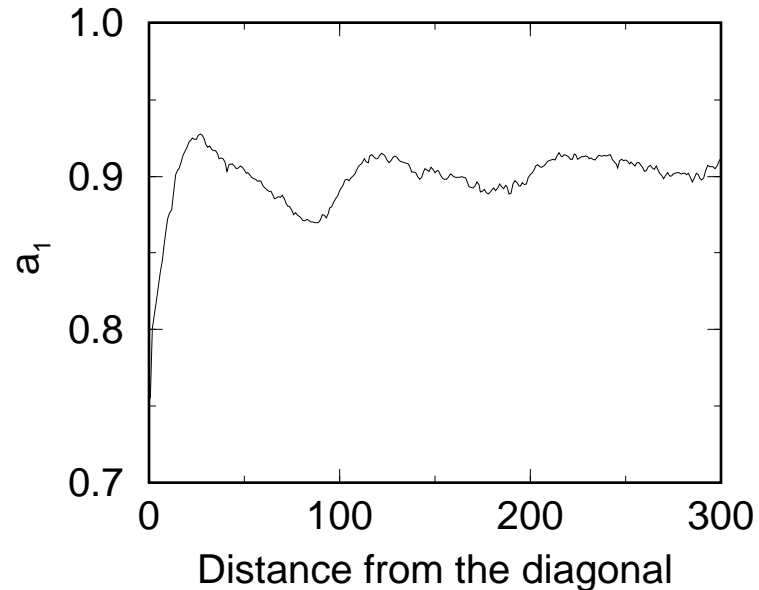


Fig. 4(b)

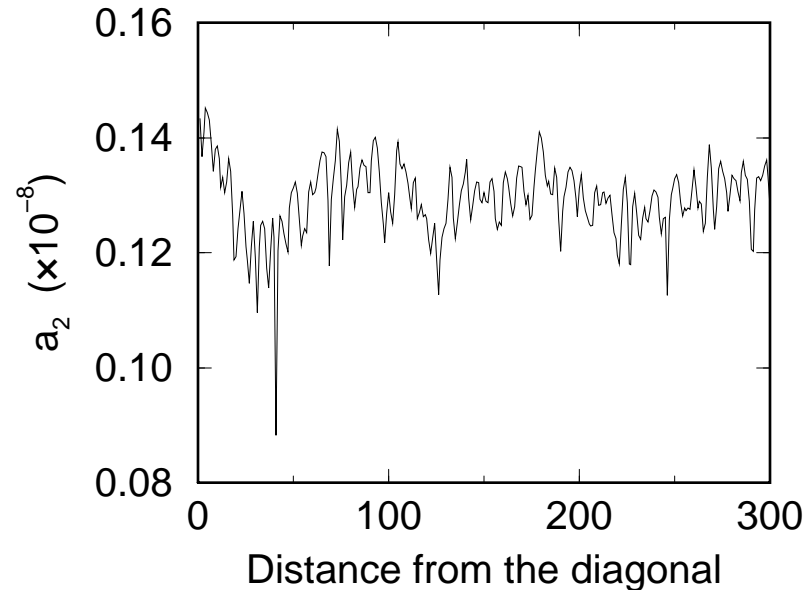


Fig. 4(c)

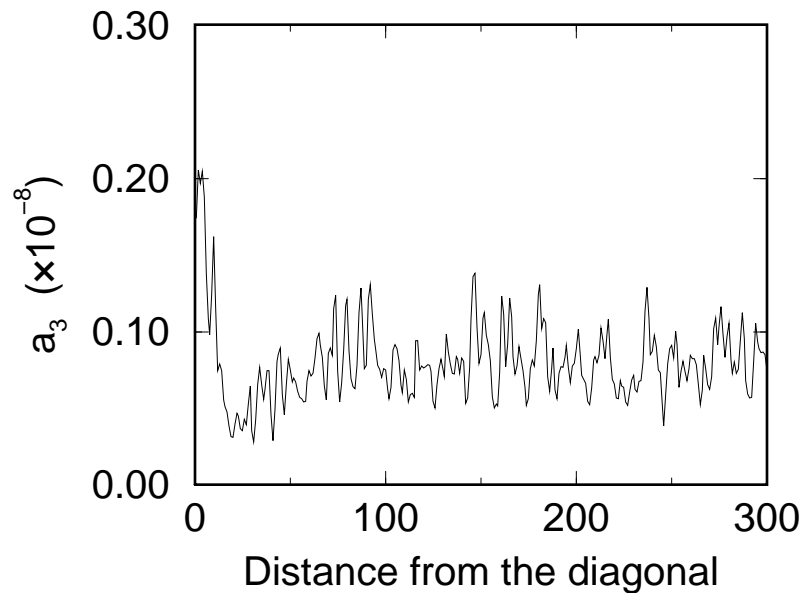


Fig. 4(d)

